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D-optimal design is unique. The design matrix of a D-optimal design is diagonal for a linear response surface. This implies that the design variables are uncorrelated and that there are no confounding effects and interactions between them. D-optimal designs for quadratic response are not orthogonal.

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OPTIMAL AIRCRAFT DESIGN METHODS

BY

RAM BACHAN RAM

FINAL REPORT
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FOR THE U.S. AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

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DEPARTMENT OF MATHEMATICAL SCIENCES
STATE UNIVERSITY OF NEW YORK
COLLEGE AT ONEONTA
ONEONTA, N.Y. 13820

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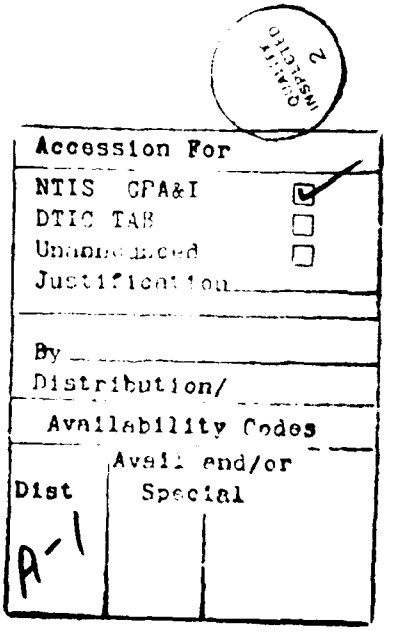


PREFACE

This technical report summarizes a study effort performed at Air Force Flight Dynamics Laboratory, Wright-Patterson Air Force Base, Ohio, under a Mini-Grant AFOSR-78-3615 from the Air Force Office of Scientific Research.

Dr. Joseph Bram, Directorate of Mathematical and Information Sciences was the Air Force Program Manager.

The Research Foundation of the State University of New York through the Local Office of Grants Administration at the State University College, Oneonta, monitored the administrative details of the grant.

SUMMARY

Study Objectives

The objectives to be pursued under this grant were to conduct analytical and application oriented (especially to aircraft industry) study of D-optimal design. The analytical study was aimed, partly, at answering questions such as:

"How does D-optimal design fare with respect to such properties as the uniqueness and orthogonality of the design, confounding of effects, interactions between the variables for linear and quadratic responses?"

The purpose of the application oriented effort was to demonstrate the application of the analytical results obtained to a typical Ground Attack Mission Profile and, independently, to a three-dimensional design space to select input conditions for an aircraft sizing program.

The computer-aided D-optimal Design Program was supplied to the Design group at Flight Dynamics Laboratory, Wright-Patterson Air Force Base, with the request to run the program and obtain the simulated values of the various responses so that further statistical analysis and a sensitivity analysis on the performance functions in a region of aircraft designs encompassing the optimum combinations of engine/airframe variables could be carried out and the validity of the theoretical results could be verified and confirmed.

This application oriented objective of the study including statistical and sensitivity analysis could not be fulfilled because of the frustrating noncooperation of the Design group in supplying the requested data. The requested simulated values have not been received even as of to-day (perhaps they will never be supplied by the Design group!).

1. INTRODUCTION

When engine cycles and airframe concepts are analytically integrated to define an airplane system, the engine and airframe subsystems or elements interact with one another. Engine physical characteristics affect the size, shape, weight and balance of the airframe. Airframe characteristics affect the installed performance of the propulsion system. If engines and airframe are to be properly integrated, element interactions, as well as isolated characteristics must be taken into account.

Engine/airframe interactions must be exploited in preliminary system design studies. Proper exploitation of subsystem interactions can only be accomplished by freeing design variables and allowing them to adjust to levels which satisfy requirements on the system and compatibility demands on one another.

Advanced engine cycle concepts add a new dimension of complexity to analytical engine/airframe integration. It is inconceivable that integration could be properly accomplished traditionally, when performance characteristics of a new, advanced engine cycle are not known completely. Furthermore, mission requirements are generally complex, very demanding, and unfamiliar. The systems which must satisfy these requirements are equally complex. To be as effective as possible, every advantage must be taken in the design of an optimum system. Free, interactive subsystem integration becomes a requirement.

Free design means all important design parameters are free to attain an optimum, system compatable value. For known airframe concepts this means at least four or five parameters must be examined. Current engine cycles have three or four and advanced cycles could add an additional two or three. So the analytical system integration problem concerns itself with from nine to twelve design parameters.

Evaluation of installed and integrated performance of advanced engine concepts requires estimation of the effects of these independent design parameters. This is accomplished through parametric perturbation of engine and airframe design variables such as cycle pressure ratio, turbine temperature, bypass ratio, engine size, wing loading, aspect ratio, thickness-to-chord ratio, etc. Their effects are expressed as values of a set of airplane performance indicators or response functions, such as range, take-off gross weight, fuel consumption, etc. If the effects of the design variables are to be estimated by manually interpolating from the function values at representative data points in a multi-dimensional problem, gross simplifications have to be made in the analysis in order to avoid large expenditures in engineering and computer time.

This usually results in only partial evaluation of the relevant effects of design variables on installed engine performance in an airplane. Even at that, the engineering time in both manhours and flowtime, as well as the computer resources required to develop the necessary data points, are prohibitive.

Therefore, in order that all the relevant design parameters in an engine/airframe concept can be analyzed, a very wide scope of engine and airframe configurations can be evaluated, and that engineering and computer resources can be cut by as much as 20%, the aircraft designers have developed a comprehensive airframe/engine screening methodology. The mathematical elements in the methodology are directed to the efficient identification of optimal combinations of engine and airframe variables (design). Optimality is defined as the process of minimizing (or maximizing) one system performance function, like takeoff gross weight, while constraining other functions, like takeoff distance, to be below (or above) a specified value. The methodology is based on advanced statistical and mathematical optimization procedures which allow maximum information to be

derived from a minimum amount of data. The procedures include statistical experimental design, regression surface fitting of engine/airframe design response function, surface fit evaluation, optimization and sensitivity analysis.

The screening process is formulated as an optimum design problem, in which a cost function (such as takeoff gross weight) is minimized subject to constraints on other response functions. The choice of algorithms for minimization with constraints may depend on many factors including whether or not derivatives, $\frac{\partial f_i}{\partial x_j}$, of the performance functions f_i with respect to design variables, x_j, are available. Gradient-directed search techniques are generally more efficient than minimization techniques which use function values only, with no derivatives (Reference 1). However, gradients may be unavailable except at great expense in terms of computer run time or the time in manhours required to supply partial derivative calculations in algorithmic form for the computer, since the ultimate functional expressions of the performance functions which generate the function values at each design point are not known in analytical form.

In order that one can save on computer run time and still be able to use an efficient gradient-directed search method, the complicated unknown performance measure functions are approximated by simple functions, for which the derivatives are easy to express analytically for the computer. These approximating functions are referred to as surface fits, since they approximate the n-dimensional surface defined in (n+1) dimensional space by a function of n variables. These approximating functions are readily expressed analytically, since they are chosen to have some elementary form, such as a polynomial.

Surface fit approximating functions make partial derivatives available in analytical form. This makes possible the direct use of a gradient-

based minimization method and results in economical optimization runs on the computer. This in turn alleviates the problem of approximation error in a region near the optimum, for this region can be explored by re-optimizing with the cost function constrained to stay within a specified cost-increase tolerance.

The coefficients for the polynomial approximating functions are obtained by using least squares regression. A surface fit approximation is formed for the hypersurface representing each response function in the multi-dimensional space of the n-design variables. Data values for the performance functions which are to be used in an engine/airframe screening evaluation are obtained at preselected combinations of design parameter values.

Additional data are used to further evaluate the validity of the approximations so obtained. Finally, the surface fit functional equations are used by the optimization/sensitivity analysis program to find a region in design space which has maximal productivity of good airplane designs.

Hence the screening methodology consists of four main steps. These are, in order of occurrence in the screening procedure:

1. The data selector step
2. The surface fit procedure
3. Evaluation of the surface fit
4. The optimization and sensitivity analysis.

These four steps precede the final evaluation of designs in the selected optimal region by the engine cycle matching and performance matching programs. The final evaluation provides direct simulation results at the design parameter combinations which have been selected in optimization/sensitivity analysis. Obviously, the validity of the results of the optimization and sensitivity analysis depends heavily on the

accuracy of the surface fit approximation procedure. For this reason, the data which is to be used in the surface fit procedure must be selected with care.

2. EXPERIMENTAL DESIGN

The search for an effective means of selecting the combinations of values for the engine/airframe design variables which are to be used for surface fit data involves the field of experimental design. Design variables are quantities such as BPR or W/S which may be varied independently as input to the engine cycle matching and performance simulation programs to obtain as output the values of certain response functions (e.g., TOGW). These functions are a measure of the performance of a hypothetical airplane design which is specified by a particular combination of values of the design variables.

Experimental design, on the other hand, refers to the design of an experiment to gather and evaluate data. Here, the data are the values of the performance functions corresponding to each of the aircraft designs which are specified by the design selector. The surface fit of approximating functions to these data involves the evaluation phase of the experiment. The approximating functions are to be used to predict the performance of airplane designs for which no data has been obtained.

These predicted performance function values, which are used by the optimization program, will be only as valid as the surface fit results. The experimental design specifies the airplane design combinations to be used in getting data values for the performance functions. It also specifies the analytical form which the surface fit approximating functions are to have. Hence, the validity of the surface fit results depends on choosing a good experimental design. But, what is a "good" experimental design?

In order to answer this question satisfactorily we need now to introduce the concept of a regression model which will, in turn be used to explain the concepts leading to the desirable properties of a "good" experimental design.

3. MODEL AND NOTATION

The set of points $P = (x_1, x_2, \ldots x_n)$ at which runs can be made is called the n-dimensional factor space. We assume that at a given point of the factor space only one quantity can be measured. Let $y_1, y_2, \ldots y_N$ be the results of observations at the points $P_1, P_2, \ldots, P_N$ of the factor space. In other words, y_j is the value of the response variable in the j^{th} trial. We consider the model

(1) $$y_j = f'(\underline{x}_j)\underline{\beta} + \varepsilon_j , \qquad j = 1, 2, \ldots, N$$

which we express in matrix notation as

(2) $$\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$$

where

(3) $\underline{Y} = (y_1, y_2, \ldots y_N)'$ is an N x 1 vector of observations,

(4) $\underline{X} = \left(f'(\underline{x}_1), f'(\underline{x}_2), \ldots, f'(\underline{x}_N)\right)'$ is an N x K matrix, $K = \frac{(n+1)(n+2)}{2}$

(5) $\underline{\beta} = (\beta_0; \beta_{11}, \beta_{22}, \ldots \beta_{nn}; \beta_1, \ldots, \beta_n; \beta_{12}, \ldots, \beta_{1n}, \beta_{23}, \ldots, \beta_{n-1,n})'$

is a K x 1 vector of unknown parameters,

(6) $\underline{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_N)'$ is an N x 1 vector of independently and identically distributed random variables ε_j with mean $E(\varepsilon_j) = 0$ and variance $V(\varepsilon_j) = \sigma^2$.

$\underline{x}_j$ denotes the value of the n x 1 vector $\underline{x} = (x_1, x_2, \ldots, x_n)'$ of predictor variables x_i at the point P_j of the factor space.

$f(\underline{x}_j)$ is a p x 1 vector which depends on the form of the response function assumed.

Based on their past experience with the performance function data, aerospace corporations have been using quadratic forms for the approximating functions. Quadratic forms are used as the baseline surface-fit function. In case these fail to provide good approximations to the performance function data values, other functional forms can be tried.

These might include combinations of higher order polynomials and exponential functions. In the following discussions the type of approximating functions will be assumed to be a quadratic polynomial so that the transpose $f'(\underline{x}_j)$ of the $p \times 1$ vector $f(\underline{x}_j)$ is given by

$$(7)\quad f'(\underline{x}_j) = \left(1;\ x_{j1}^2, \ldots, x_{jn}^2;\ x_{j1}, \ldots, x_{jn};\ x_{j1}x_{j2}, \ldots, x_{j1}x_{jn}, x_{j2}x_{j3}, \ldots, x_{jn-1}x_{jn}\right)$$

x_{ji} is the value of the independent variable x_i in the j^{th} trial.

Substituting for $f'(\underline{x}_j)$ from (7) in (4) the matrix $\underline{X}$ becomes

$$(8)\quad \underline{X} = \begin{bmatrix} 1 & x_{11}^2 \cdots x_{1n}^2 & x_{11} \cdots x_{1n} & x_{11}x_{12} \cdots x_{11}x_{1n} & x_{12}x_{13} \cdots x_{1n-1}x_{1n} \\ 1 & x_{21}^2 \cdots x_{2n}^2 & x_{21} \cdots x_{2n} & x_{21}x_{22} \cdots x_{21}x_{2n} & x_{22}x_{23} \cdots x_{2n-1}x_{2n} \\ 1 & x_{N1}^2 \cdots x_{Nn}^2 & x_{N1} \cdots x_{Nn} & x_{N1}x_{N2} \cdots x_{N1}x_{Nn} & x_{N2}x_{N3} \cdots x_{Nn-1}x_{Nn} \end{bmatrix}$$

Substituting for $\underline{X}$ from (8), for $\underline{\beta}$ from (5), for $\underline{\varepsilon}$ from (6), and for $\underline{Y}$ from (3) in Eq. (2), we obtain

$$(9)\quad \begin{bmatrix} y_1 \\ \vdots \\ y_j \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} \beta_0 + \sum_{i=1}^{n} \beta_{ii} x_{1i}^2 + \sum_{i=1}^{n} \beta_i x_{1i} + \sum_{h=1}^{n-1} \sum_{\substack{i=2 \\ h<i}}^{n} \beta_{hi} x_{1h} x_{1i} + \varepsilon_1 \\ \vdots \\ \beta_0 + \sum_{i=1}^{n} \beta_{ii} x_{ji}^2 + \sum_{i=1}^{n} \beta_i x_{ji} + \sum_{h=1}^{n-1} \sum_{\substack{i=2 \\ h<i}}^{n} \beta_{hi} x_{jh} x_{ji} + \varepsilon_j \\ \vdots \\ \beta_0 + \sum_{i=1}^{n} \beta_{ii} x_{Ni}^2 + \sum_{i=1}^{n} \beta_i x_{Ni} + \sum_{h=1}^{n-1} \sum_{\substack{i=2 \\ h<i}}^{n} \beta_{hi} x_{Nh} x_{Ni} + \varepsilon_N \end{bmatrix}$$

This matrix equation yields a system of N equations

$$(10)\quad y_j = \beta_0 + \sum_{i=1}^{n} \beta_{ii} x_{ji}^2 + \sum_{i=1}^{n} \beta_i x_{ji} + \sum_{h=1}^{n-1} \sum_{\substack{i=2 \\ h<i}}^{n} \beta_{hi} x_{jh} x_{ji} + \varepsilon_j, \qquad j = 1, 2, \ldots, N$$

which is the same as Eq. (1) after substituting for $f'(\underline{x}_j)$ from (7).

Denoting by $\underline{X}'$ the transpose of the matrix $\underline{X}$, the $K \times K$ symmetric matrix $\underline{X}'\underline{X}$ is called the <u>information matrix</u>. Using (8) we get

(11) $$\underline{X}'\underline{X} = \begin{bmatrix}
N & \sum_{j=1}^{N} x_{j1}^2 & \sum x_{j2}^2 & \cdots & \sum x_{jn}^2 & \sum x_{j1} & \sum x_{j2} & \cdots & \sum x_{jn-1}x_{jn} \\
\sum x_{j1}^2 & \sum x_{j1}^4 & \sum x_{j1}^2 x_{j2}^2 & \cdots & \sum x_{j1}^2 x_{jn}^2 & \sum x_{j1}^3 & \sum x_{j1}^2 x_{j2} & \cdots & \sum x_{j1}^2 x_{jn-1}x_{jn} \\
\sum x_{j2}^2 & \sum x_{j2}^2 x_{j1}^2 & \sum x_{j2}^4 & \cdots & \sum x_{j2}^2 x_{jn}^2 & \sum x_{j2}^2 x_{j1} & \sum x_{j2}^3 & \cdots & \sum x_{j2}^2 x_{jn-1}x_{jn} \\
\vdots & & & & & & & & \vdots \\
\sum x_{jn}^2 & \sum x_{jn}^2 x_{j1}^2 & \sum x_{jn}^2 x_{j2}^2 & \cdots & \sum x_{jn}^4 & \sum x_{jn}^2 x_{j1} & \sum x_{jn}^2 x_{j2} & \cdots & \sum x_{jn}^3 x_{jn-1} \\
\sum x_{j1} & \sum x_{j1}^3 & \sum x_{j1}x_{j2}^2 & \cdots & \sum x_{j1}x_{jn}^2 & \sum x_{j1}^2 & \sum x_{j1}x_{jn} & \cdots & \sum x_{j1}x_{jn-1}x_{jn} \\
\sum x_{j2} & \sum x_{j2}x_{j1}^2 & \sum x_{j2}^3 & \cdots & \sum x_{j2}x_{jn}^2 & \sum x_{j2}x_{j1} & \sum x_{j2}^2 & \cdots & \sum x_{j2}x_{jn-1}x_{jn} \\
\vdots & & & & & & & & \vdots \\
\sum x_{jn} & \sum x_{jn}x_{j1}^2 & \sum x_{jn}x_{j2}^2 & \cdots & \sum x_{jn}^3 & \sum x_{jn}x_{j1} & \sum x_{jn}x_{j2} & \cdots & \sum x_{jn-1}x_{jn}^2 \\
\sum x_{j1}x_{j2} & \sum x_{j1}^3 x_{j2} & \sum x_{j1}x_{j2}^3 & \cdots & \sum x_{j1}x_{j2}x_{jn}^2 & \sum x_{j1}^2 x_{j2} & \sum x_{j1}x_{j2}^2 & \cdots & \sum x_{j1}x_{j2}x_{jn-1}x \\
\vdots & & & & & & & & \\
\sum x_{j1}x_{jn} & \sum x_{j1}^3 x_{jn} & \sum x_{j1}x_{j2}^2 x_{jn} & \cdots & \sum x_{j1}x_{jn}^3 & \sum x_{j1}^2 x_{jn} & \sum x_{j1}x_{j2}x_{jn} & \cdots & \sum x_{j1}x_{jn-1}x \\
\sum x_{j2}x_{j3} & \sum x_{j1}^2 x_{j2}x_{j3} & \sum x_{j2}^3 x_{j3} & \cdots & \sum x_{j2}x_{j3}x_{jn}^2 & \sum x_{j1}x_{j2}x_{j3} & \sum x_{j2}^2 x_{j3} & \cdots & \sum x_{j2}x_{j3}x_{jn} \\
\vdots & & & & & & & & \\
\sum x_{jn-1}x_{jn} & \sum x_{jn-1}x_{jn}x_{j1}^2 & \sum x_{jn-1}x_{jn}x_{j2}^2 & \cdots & \sum x_{jn-1}x_{jn}^3 & \sum x_{jn-1}x_{jn}x_{j1} & \sum x_{jn-1}x_{jn}x_{j2} & \cdots & \sum x_{jn-1}^2 x_{jn}^2
\end{bmatrix}$$

Let us dentoe the $K\times 1$ vector of estimated regression coefficients $b_0;\ b_{11},\ b_{22},\cdots,\ b_{nn};\ b_1,\cdots,b_n;\ b_{12},\cdots,b_{1n},\ b_{23},\cdots,\ b_{n-1\,n}$ as $\underline{b}$:

(12) $$\underline{b} = \left(b_0\ \ b_{11}\cdots b_{nn}\ b_1\cdots b_n\ b_{12}\cdots,b_{1n}\ b_{23}\cdots\ b_{n-1\,n}\right)'$$

Then assuming that the information matrix is non-singular, the least squares estimates of the unknown parameters $\underline{\beta}$ in the regression model (2) are given by

(13) $$\underline{b} = \left(\underline{X}'\underline{X}\right)^{-1}\underline{X}'\underline{Y}$$

The variance-covariance matrix of $\underline{b}$ is

(14) $$V(\underline{b}) = \sigma^2\left(\underline{X}'\underline{X}\right)^{-1}$$

At any point $\underline{x}$ of the experimental region χ, the predicted response is

(15) $$\hat{Y}(\underline{x}) = f'(\underline{x})\,\underline{b}$$

with variance

$$V\left[\hat{\underline{Y}}(\underline{x})\right] = \sigma^2 \underline{f}'(\underline{x})\left(\underline{X}'\underline{X}\right)^{-1}\underline{f}(\underline{x}) \tag{16}$$

4. REPARAMETERIZATION

Least squares results tend to be sensitive to rounding of data in intermediate stages of calculations. When the number of independent variables is small - say three or less - roundoff effects can be controlled by carrying a sufficient number of digits in intermediate calculations. But this expedient becomes increasingly inefficient as the number of independent variables becomes larger. Roundoff errors tend to enter into least squares calculations primarily when the inverse of $\underline{X}'\underline{X}$ is taken. Of course, any errors in $\left(\underline{X}'\underline{X}\right)^{-1}$ may be magnified when calculating $\underline{b}$ (see Eq. 13) or making other subsequent calculations (see Eqs. 14, 16). The danger of serious roundoff errors in $\left(\underline{X}'\underline{X}\right)^{-1}$ is particularly great when the elements of $\underline{X}'\underline{X}$ differ substantially in order of magnitude. A solution for this condition is to transform the variables and thereby reparameterize the regression model. If ξ_i denotes a natural independent variable and x_i the corresponding transformed variable, then the transformation

$$x_i = \frac{\xi_i - \frac{1}{2}\left(\xi_{i,\max} + \xi_{i,\min}\right)}{\frac{1}{2}\left(\xi_{i,\max} - \xi_{i,\min}\right)}, \tag{17}$$

where $\xi_{i,\max}$ = maximum value of ξ_i,

$\xi_{i,\min}$ = minimum value of ξ_i,

makes the transformed variables to fall between -1 and +1, so that the calculation of the inverse matrix becomes much less subject to roundoff errors due to dissimilar orders of magnitudes than with the original variables. The transformed variables x_i are called the normalized form of the natural variables ξ_i, $i=1,\ldots,n$. Henceforth, we assume that the independent variables x_i appearing in this work are all normalized so that $-1 \le x_i \le 1$.

Further, the regression coefficients, even in the reparameterized model, are affected by the spacing of the independent variables, which may be quite arbitrary. It is desirable, therefore, to scale the factors uniformly, and we shall do this by imposing the following restrictions upon the values of the independent variables:

$$\sum_{j=1}^{N} x_{ji} = \sum_{j} x_{ji}^3 = \sum_{j} x_{jh}\, x_{ji} = \sum_{j} x_{jh}^2\, x_{ji} = \sum x_{jh}^3\, x_{ji} = \sum x_{jh}^2\, x_{ji}\, x_{ik} =$$
$$= \sum_{j} x_{jh}\, x_{ji}\, x_{il} = \sum x_{jh}\, x_{ji}\, x_{jl}\, x_{jk} = 0$$

(18)

$$\sum_{j} x_{ji}^2 = a\,, \quad \sum x_{jh}^2\, x_{ji}^2 = c\,, \quad \sum_{j} x_{ji}^4 = c + d\,.$$

The matrix $\underline{X}'\underline{X}$ now takes a convenient form:

$$\underline{X}'\underline{X} = \begin{bmatrix} \begin{pmatrix} N & a & a & a & \cdots & a \\ a & c+d & c & c & \cdots & c \\ a & c & c+d & c & \cdots & c \\ \cdot & \cdot & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & \cdot & & \\ a & c & c & c & \cdots & c+d \end{pmatrix} & \begin{matrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & & 0 \\ 0 & 0 & & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & & 0 \end{matrix} & \begin{matrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & & 0 \\ 0 & 0 & & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & & 0 \end{matrix} \\ \begin{matrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \cdot & \cdot & & & & \\ \cdot & \cdot & & & & \\ \cdot & \cdot & & & & \\ 0 & 0 & 0 & 0 & & 0 \end{matrix} & \begin{pmatrix} a & 0 & \cdots & 0 \\ 0 & a & \cdots & 0 \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ 0 & 0 & \cdots & a \end{pmatrix} & \begin{matrix} 0 & 0 \\ 0 & 0 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ 0 & 0 \end{matrix} \\ \begin{matrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \cdot & \cdot & & & & \\ \cdot & \cdot & & & & \\ \cdot & \cdot & & & & \\ 0 & 0 & 0 & 0 & & 0 \end{matrix} & \begin{matrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ 0 & 0 & \cdots & 0 \end{matrix} & \begin{pmatrix} c & 0 & \cdots & 0 \\ 0 & c & \cdots & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & \cdots & c \end{pmatrix} \end{bmatrix} \tag{19}$$

$$\underline{X}'\underline{X} = \begin{bmatrix} N & a\underline{1}_n' & \underline{0} & \underline{0} \\ a\underline{1}_n & c\underline{J}_n + d\underline{I}_n & \underline{0} & \underline{0} \\ \underline{0} & \underline{0} & a\underline{I}_n & \underline{0} \\ \underline{0} & \underline{0} & \underline{0} & C\underline{I}_{\binom{n}{2}} \end{bmatrix} \tag{20}$$

where $\underline{1}_n = (1 \quad 1 \ldots 1)'$ is an n x 1 vector, $\underline{J}_n$ is a square matrix of order n with every element 1, and $\underline{I}_n$ is a unit matrix of order n.

The inverse $(\underline{X}'\underline{X})^{-1}$, when it exists, is a similarly patterned matrix

$$(\underline{X}'\underline{X})^{-1} = \begin{bmatrix} p & q\underline{1}_n' & \underline{0} & \underline{0} \\ q\underline{1}_n & s\underline{J}_n + t\underline{I}_n & \underline{0} & \underline{0} \\ \underline{0} & \underline{0} & a^{-1}\underline{I}_n & \underline{0} \\ \underline{0} & \underline{0} & \underline{0} & c^{-1}\underline{I}_{\binom{n}{2}} \end{bmatrix} \tag{21}$$

Taking the product $(\underline{X}'\underline{X})(\underline{X}'\underline{X})^{-1} = I_K$ gives a set of five consistent equations in the four unknowns p, q, s and t.

$$Np + naq = 1 \tag{22}$$

$$Nq + a(ns + t) = 0 \tag{23}$$

$$ap + q(nc + d) = 0 \tag{24}$$

$$aq + ds + ct + ncs = 0 \tag{25}$$

$$dt = 1 \tag{26}$$

The last equation gives $t = 1/d$. Eliminating t from Eqs. (22) and (24) gives

$$s = -\frac{(a^2 - Nc)q}{ad}$$

and solving Eqs. (21) and (23) gives

$$ap = -(nc + d)q$$

and

$$q = -a/[N(nc + d) - na^2]$$

If we now write

$$[d\{N(nc + d) - na^2\}]^{-1} = A$$

these solutions become

$$p = d(nc + d)A, \quad q = -adA, \quad s = (a^2 - Nc)A, \text{ and } t = \frac{1}{d}.$$

Using the form (21) of the inverse matrix $(\underline{X}'\underline{X})^{-1}$ of the information

matrix, the variance-covariance matrix (14) becomes

$$V(\underline{b}) = \begin{bmatrix} p\sigma^2 & \sigma^2 q \underline{1}'_n & \underline{0} & \underline{0} \\ \sigma^2 q \underline{1}_n & \sigma^2 s \underline{J}_n + \sigma^2 t \underline{I}_n & \underline{0} & \underline{0} \\ \underline{0} & \underline{0} & \sigma^2 \bar{a}^1 \underline{I}_n & \underline{0} \\ \underline{0} & \underline{0} & & \sigma^2 C^{-1} \underline{I}_{\binom{n}{2}} \end{bmatrix} \tag{27}$$

It would be convenient if we could choose the design points in such a way that cov $(b_0, b_{hh}) = 0$ for all h, and cov $(b_{hh}, b_{ii}) = 0$ for all h, i, $h \neq i$. The first condition cannot be satisfied, for we have

$$\text{cov}\ (b_0, b_{hh}) = \sigma^2 q = -\ adA\sigma^2$$

and $a>0$, $d>0$, $A\neq 0$. Hence, $q\neq 0$ and the covariance cannot be made to vanish. On the other hand,

$$\text{cov}\ (b_{hh}, b_{ii}) = s\sigma^2 = (a^2 - Nc)\ A\sigma^2$$

and a necessary and sufficient condition for this to vanish is that

$$a^2 - Nc = 0$$

It is customary to call the property

$$\text{cov}\ (b_{hh}, b_{ii}) = 0 \tag{28}$$

the <u>orthogonality property for quadratic response surface designs</u>, and

$$a^2 = Nc \tag{29}$$

the <u>orthogonality condition for quadratic response surface designs</u>.

5. DESIRABLE PROPERTIES OF A GOOD EXPERIMENTAL DESIGN

Now we are in a position to answer the question raised in Section 2 as to what characterizes a "good" experimental design. These characteristics are described below.

(a) <u>Non-singular information matrix</u>. The experimental design should allow choice of such points in the factor space χ that under the information matrix non-singular allowing the normal equations to yield least squares estimates $\underline{b}$ of the unknown parameters $\underline{\beta}$ (see Eq. 13). The number of such points in χ should be kept to a minimum in order to make the process more cost effective. For a n-dimensional design

of order d, this minimum number is $\binom{n+d}{d}$. A design matrix $\underline{X}$ (see Eq. 8) of a n-dimensional design of order d is said to be saturated if it has exactly $\binom{n+d}{d}$ linearly independent rows.

(b) No confounding of the effects of different terms in the surface-fit equation. Confounding is the degree to which the effects of the terms in the surface-fit equation are (pairwise) confused with one another in the measurements of the values y_k obtained from the data. Suppose, for example, that two independent design variables x_i and x_j $(i \neq j)$ are very highly correlated in the data. This will cause the value of the linear correlation coefficient r_{ij} to be close to +1 or -1. This implies that the measured values y_k are, as far as x_i and x_j are concerned, almost a function of a single variable. It will be hard to separate the variation in y_k due to x_i from the variation due to x_j using the data from the design points specified in the experimental design. Instead, design points $\underline{x}_k$ should be selected in such a way that $r_{ij} = 0$ ideally (though it is enough that r_{ij} lie within a confidence band of values near 0). This renders the design variables $x_1, x_2, \ldots, x_n$ statistically as well as functionally independent.

When the surface-fit equation is linear in the design variables $x_1, x_2, \ldots, x_n$ and if these design variables are functionally independent, then the matrix $\underline{X}'\underline{X}$ is non-singular and the model coefficients β_i, have the smallest variance when $\underline{X}'\underline{X}$ is diagonal. Indeed, consider the regression model for a linear response surface

$$y_j = \beta_0 + \sum_{i=1}^{n} \beta_i x_{ji} + \varepsilon_j \,, \quad j = 1, 2, \ldots, N \tag{29}$$

which we express in matrix notation as

$$\underline{Y} = \underline{X}\,\underline{\beta} + \underline{\varepsilon} \tag{30}$$

where

$$(31)\qquad \underline{X} = \begin{bmatrix} 1 & x_{11} \cdots x_{1n} \\ 1 & x_{21} \cdots x_{2n} \\ \vdots & \\ 1 & x_{N1} \cdots x_{Nn} \end{bmatrix}, \quad \underline{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \quad \underline{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_n \end{bmatrix}, \quad \underline{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_N \end{bmatrix}$$

The information matrix $M = \underline{X}'\underline{X}$ is

$$(32)\qquad M = \begin{bmatrix} N & \sum_{j=1}^{N} x_{j1} & \sum_{j=1}^{N} x_{j2} & \cdots & \sum_{j=1}^{N} x_{jn} \\ \sum x_{j1} & \sum x_{j1}^2 & \sum x_{j1}x_{j2} & \cdots & \sum x_{j1}x_{jn} \\ \sum x_{j2} & \sum x_{j2}x_{j1} & \sum x_{j2}^2 & \cdots & \sum x_{j2}x_{jn} \\ \vdots & & & & \\ \sum x_{jn} & \sum x_{jn}x_{j1} & \sum x_{jn}x_{j2} & \cdots & \sum x_{jn}^2 \end{bmatrix}$$

Then it can be shown (see pp. 109-110 of reference [1]) that

$$(33)\qquad V(b_p) = \frac{\sigma^2}{N}\left(1 + \frac{Q}{|M|}\right),$$

where Q is a positive definite form in the nondiagonal elements of M.

Since $|M| > 0$, $\frac{Q}{|M|} \geq 0$

$\frac{Q}{|M|} = 0$ iff nondiagonal elements of M are zero; that is,

M is a diagonal matrix.

$$(34)\qquad M \text{ diagonal} \Rightarrow \text{Var}(b_p) = \frac{\sigma^2}{N} = \min \text{Var}(b_p)$$

Adopting the following coding for the design variables

$$(35)\qquad x_{ji} = \frac{\xi_{ji} - \bar{\xi}_i}{S_i}$$

where ξ_{ji} denotes the actual value of the j^{th} level of the i^{th} variable, $\bar{\xi}_i$ is the average of the levels of the i^{th} variable, and

$$(36)\qquad S_i^2 = \frac{\sum_{j=1}^{N} (\xi_{ji} - \bar{\xi}_i)^2}{N}$$

we get

$$(37)\qquad \sum_{j=1}^{N} x_{ji}^2 = N$$

and

$$(38)\quad M = \begin{bmatrix} N & 0 & 0 & \cdots & 0 \\ 0 & N & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ N & 0 & 0 & \cdots & N \end{bmatrix}$$

In this case (i.e., when M is given by (37))the variance covariance matrix of $\underline{b}$

$$(39)\quad V(\underline{b}) = \sigma^2 M^{-1}$$

takes the form

$$(40)\quad \begin{bmatrix} V(b_0) & cov(b_0,b_1) & \cdots & cov(b_0,b_n) \\ cov(b_1,b_0) & V(b_1) & \cdots & cov(b_1,b_n) \\ \vdots & & & \\ cov(b_n,b_0) & cov(b_n,b_1) & \cdots & V(b_n) \end{bmatrix} = \begin{bmatrix} \frac{\sigma^2}{N} & 0 & 0 \cdots 0 \\ 0 & \frac{\sigma^2}{N} & 0 \cdots 0 \\ \vdots & & \vdots \\ 0 & 0 & 0 \cdots \frac{\sigma^2}{N} \end{bmatrix}$$

$$(41)\quad \Rightarrow \quad cov(b_h, b_i) = 0 \,, \quad h \neq i$$

$\Rightarrow$

1. X_h and X_i are uncorrelated,
2. No confounding effects, and
3. No interactions between the design variables.

When the response surface is approximated by a polynomial of degree higher than the first, the quantities $X_0; X_1, X_2, \ldots, X_n; X_1^2, \ldots, X_n^2$; X_1X_2, ... are not all functionally independent and a diagonal moment matrix is impossible of attainment. Hence even there is no assurance that the matrix $\underline{X}'\underline{X}$ is non-singular.

(c) Orthogonal design. Experimental designs for which the information matrix $\underline{X}'\underline{X}$ can be diagonalized (see Eq. (38)) for linear response surface), and thus, the coefficients in the surface fit equation are uncorrelated with one another (see Eq. (41)) for the linear response),

are called orthogonal designs. For the quadratic response represented by the model in Eq. 10, orthogonality of the design implies $Cov(b_{ii}, b_{nn}) = 0$ (see Eq. 28). The prediction uncertainty, which is measured by the variance, for function values and derivatives using surface fit equations can be kept relatively low by the use of orthogonal designs. Indeed, there is a certain amount of uncertainty in the estimation of the vector $\underline{b}$ of model coefficients (see Eqs. 5 and 31). This uncertainty is determined by the choice of experimental design, as seen from the variance-covariance matrix (14) and the Eqs. (33) and (40). The uncertainty in the estimation of model coefficients causes an uncertainty in the prediction of function values at any point $\underline{x}$ in design space χ. Indeed, let $\underline{x}$ be a specified 1 x n vector whose elements are of the same form as a row of the matrix $\underline{X}$ (see Eq. 8). Then $\hat{y}_o$ is the value predicted at $\underline{x}_o$ by the regression equation and has variance

$$V(\hat{y}_o) = \underline{x}_o' V(\underline{b}) \underline{x}_o$$

This uncertainty can strongly affect the sensitivity analysis at an optimum $\underline{x}^*$ located by the optimization method applied to the surface fit functions.

If the design is orthogonal, the prediction uncertainty for function values of responses described by a linear response surface can be reduced to a minimum because the variances of estimated model coefficients, $var(b_p)$, take minimum values in this case (see Eq. 34). This results in a better curve-fit of the approximated response to the actual response surface.

In practice, trial values for the design point combinations $(x_{j1}, x_{j2}, \cdots x_{jn})$ can always be evaluated for the above properties prior to actually using these points as input to an engine/airframe

simulator program. Design points can be added and discarded until the desired number N of points satisfying these properties is achieved. However, this is potentially a time consuming procedure unless a computer algorithm can be formulated for the process of adding and deleting large number of data points while testing the correlation coefficient r_{ij}, the matrix $\underline{X}'\underline{X}$, etc., which, on the other hand, may increase the cost factor. Therefore, a reliable a priori choice of experimental design is needed instead which may possess the above desired properties, can minimize the cost of the approximations with actual increase in accuracy, and yields a flyable aircraft. Recent investigations on experimental designs show that a considerable enhancement of the screening methodology based on the number of design points needed and the efficiencies of the designs involved can be realized. As such, ϕ_p- Optimal designs, $0 \le p \le \infty$, as proposed by Kiefer, become potential candidates for such a choice. In this report we will limit our considerations to ϕ_0- -Optimal designs, known as D-Optimal designs, only.

6. D-OPTIMAL DESIGNS

Consider the N x N information matrix

$$M(\xi) = \int_{\chi} \underline{f}'(x)\, \underline{f}(x)\, \xi(dx)$$

where N is the number of unknown parameters, ξ is the design, that is, in general, a probability measure over experimental region χ, and f is the unknown regression function $(f_1(x), \ldots, f_N(x))$. Assuming the information matrix to be non-singular, let $\lambda_1(\xi), \ldots, \lambda_N(\xi)$ denote the eigenvalues of $M(\xi)$. Define the functional $\phi_p(\xi)$ by

$$\phi_p(\xi) = \left[N^{-1} \operatorname{tr} M^{-p}(\xi)\right]^{1/p} = \left[N^{-1} \sum_{i=1}^{N} \lambda_i^{-p}(\xi)\right]^{1/p}, \qquad 0 < p < \infty$$

$$\phi_0(\xi) = \lim_{p \to 0^+} \phi_p(\xi) = \left[\det M^{-1}(\xi)\right]^{1/N}$$

$$\phi_\infty(\xi) = \lim_{p \to +\infty} \phi_p(\xi) = \max_{1 \le i \le N} \lambda_i^{-1}(\xi)$$

A ϕ_p - optimal design $\xi^{(p)}$ is one that minimizes $\phi_p(\xi)$. Thus, a ϕ_0 - optimal design minimizes $\left[\det M^{-1}(\xi)\right]^{1/N}$ which is equivalent to saying that ϕ_0 - optimal design maximizes $\det M(\xi)$. For this reason a ϕ_0 - optimal design is called D-Optimal design because it maximizes the DETERMINANT of the information matrix.

Notation. A normalized design will be denoted by ϵ and its information matrix by $M(\epsilon)$.

6.1 Some Basic Results

Linear combination of two normalized designs. Let ϵ_1 and ϵ_2 be two arbitrary normalized designs given on the closed set χ. Let each of these designs be characterized by the corresponding measure $\xi_1(x)$ and the measure $\xi_2(x)$. Then by the linear combination of these designs

$$\epsilon = (1-\alpha)\epsilon_1 + \alpha\epsilon_2 \quad , \qquad 0 < \alpha < 1, \tag{42}$$

is understood the normalized design with measure

$$\xi(x) = (1-\alpha)\xi_1(x) + \alpha\xi_2(x) \tag{43}$$

Relying directly on the definition of the information matrix, it is easy to verify the following lemma.

Lemma 1. The information matrix $M(\epsilon)$ of the normalized design $\epsilon = (1-\alpha)\epsilon_1 + \alpha\epsilon_2$ is given by

$$M(\epsilon) = (1-\alpha)M(\epsilon_1) + \alpha M(\epsilon_2) \tag{44}$$

It is known from the theory of positive-definite matrices that

If A and B are positive-definite matrices of order m, $A \neq B$, and $0 < \alpha < 1$, then

$$|\alpha A + (1-\alpha)B| > |A|^{\alpha}\,|B|^{1-\alpha} \tag{45}$$

Using (45) it is trivial to verify the following lemma.

Lemma 2. The function $\log|M(\epsilon)|$ of the information matrix $M(\epsilon)$ defined by (44) is a strictly concave function.

That is,

$$\log|M(\epsilon)| > (1-\alpha)\log|M(\epsilon_1)| + \alpha\log|M(\epsilon_2)| \tag{46}$$

Using this lemma it is easy to prove the following theorem.

Theorem 1. If ϵ_1 and ϵ_2 are two normalized designs with distinct information matrices $M(\epsilon_1)$ and $M(\epsilon_2)$, for which $|M(\epsilon_1)| = |M(\epsilon_2)|$, then the design $\epsilon = (1-\alpha)\epsilon_1 + \alpha\epsilon_2$, $0 < \alpha < 1$ has the determinant $|M(\epsilon)| > |M(\epsilon_1)|$

Now we are in a position to prove the following important theorem.

Theorem 2. (Uniqueness of D-Optimal designs)

Let ϵ_1 and ϵ_2 be two normalized D-Optimal designs with information matrices $M(\epsilon_1)$ and $M(\epsilon_2)$. Then $M(\epsilon_1) = M(\epsilon_2)$.

Proof. Suppose, on the contrary, that $M(\epsilon_1) \neq M(\epsilon_2)$.

Construct a design $\epsilon = (1-\alpha)\epsilon_1 + \alpha\epsilon_2$, $0 < \alpha < 1$

Since ϵ_1 and ϵ_2 are D-Optimal, $|M(\epsilon_1)| = |M(\epsilon_2)|$

Hence, by Theorem 1, $|M(\epsilon)| > |M(\epsilon_1)|$

This contradicts the fact that ϵ_1 is D-Optimal. Hence the theorem follows.

Theorem 3. (Diagonal Information Matrix)

For a linear response surface the information matrix of a normalized D-Optimal design is diagonal. In other words, the D-Optimal design for a linear response surface is orthogonal.

Proof. Let ϵ^* be a normalized D-Optimal design with information matrix $M(\epsilon^*)$. Suppose $M(\epsilon^*)$ is not diagonal. Then we can construct another design $\tilde{\epsilon}$ from ϵ^* by taking the elements of $\tilde{\epsilon}$ the mirror image with respect to zero of the corresponding elements of ϵ^*. Clearly $M(\tilde{\epsilon}) \neq M(\epsilon^*)$. It is not difficult to show that $|M(\tilde{\epsilon})| = |M(\epsilon^*)|$. Now, consider the design $\epsilon = \frac{1}{2}\epsilon^* + \frac{1}{2}\tilde{\epsilon}$

By Theorem 1, for $\alpha = 1/2$,

$$|M(\epsilon)| > |M(\epsilon^*)|,$$

which contradicts the assumption that ϵ^* is D-Optimal. This contradiction proves the theorem.

6.2 D-Optimal Design for Quadratic Response

Kiefer and his collaborators, and Pesotchisky have considered ϕ_p-optimal designs for quadratic regression on such experimental regions as the q- simplex, q- dimensional ball, q-dimensional cube, etc. because these regions turn out to be much more tractable computationally and hence many results can be obtained algebraically. For the reasons pointed out in section 4 and the area of application of this effort, it will be desirable for us to consider the settings in which the design (controllable) variables are restricted to the n-dimensional cube

$$\mathcal{X} = C_n = \{(x_1, x_2, \ldots, x_n) : |x_i| \le 1, \ i = 1, 2, \ldots, n\}$$

Much of our discussion is phrased in terms of certain simple subsets of C_n, which we now define.

Barycenter of depth i. A barycenter of depth i ($0 \le i \le n$) is a point with i coordinates equal to 0 and the remaining coordinates equal to ± 1.

We denote the set of $\binom{n}{i} 2^{n-i}$ barycenters of depth i by J_i, and write $J = \bigcup_{i=0}^{n} J_i$. Thus, J_0 consists of the vertices of C_n, J_1 consists of midpoints of edges, J_2 consists of the centers of 2-dimensional cubical faces, J_n is the single center point, etc. For example,

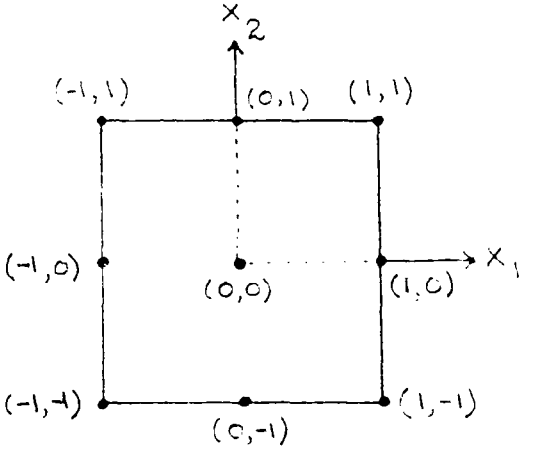
for $C_2 = \{(x_1, x_2) : |x_i| \le 1\}$, we have

$J_0 = \{(1,1), (-1,1), (1,-1), (-1,-1)\}$

$J_1 = \{(1,0), (-1,0), (0,1), (0,-1)\}$

$J_2 = \{(0,0)\}$

$J = \bigcup_{i=0}^{2} J_i = \{(1,1), (-1,1), (1,-1), (-1,-1), (1,0), (-1,0), (0,1), (0,-1), (0,0)\}$



for $C_3 = \{(x_1, x_2, x_3) : |x_i| \le 1, \ i = 1, 2, 3\}$, we have

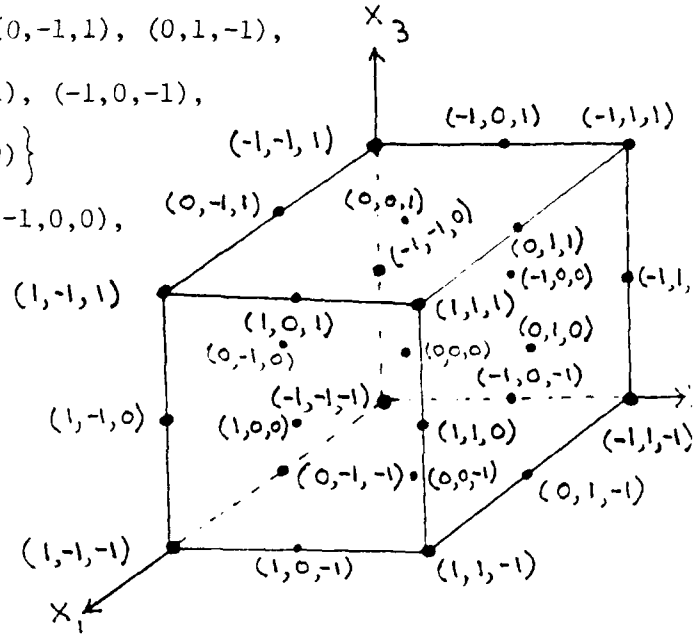
$J_0 = \{(1, 1, 1), (-1, 1, 1), (1, -1, 1), (1, 1, -1), (-1, -1, 1), (-1, 1, -1), (1, -1, -1), (-1, -1, -1)\}$

$$J_1 = \{(0,1,1),\ (1,0,1),\ (1,1,0),\ (0,-1,1),\ (0,1,-1),\ (0,-1,-1),\ (-1,0,1),\ (1,0,-1),\ (-1,0,-1),\ (-1,1,0),\ (1,-1,0),\ (-1,-1,0)\}$$

$$J_2 = \{(1,0,0),\ (0,1,0),\ (0,0,1),\ (-1,0,0),\ (0,-1,0),\ (0,0,-1)\}$$

$$J_3 = \{(0,0,0)\}$$

$$J = \bigcup_{i=0}^{3} J_i$$



The following theorems were proved by Kiefer (1960, 1974, [3], [4]) and by Farrell, Kiefer, and Walbran (1965, [5]) which allow the choice of design (controllable) variables from a simple subset of J and establish the existence of a symmetric ϕ_p- Optimum design. For the proofs of these two theorems the reader is referred to references [3], [4], [5].

Theorem 4. Every D-Optimal design is supported by a subset of J.

Theorem 5. There is a D-Optimal design that is symmetric under all permutations of coordinates and multiplication of any x_i by -1.

In the light of theorems 2, 4, and 5 we shall limit our considerations only to Symmetric D-Optimal Designs on J. Further characterizations of symmetric designs are contained in the following two theorems.

Theorem 6. Any symmetric design can be described in terms of a probability (n+1) - vector $\underline{\eta} = (\eta_0, \eta_1, \cdots, \eta_n)'$ that assigns measure $\eta_i / \binom{n}{i} 2^{n-i}$ to each point of J_i.

Theorem 7. For a symmetric D-Optimal design, there exists the simplest probability vector $\underline{\eta}$ for which only three η_i's are positive.

In the light of Theorem 7, one needs to consider D-Optimal designs of the following form only:

(i) Observations with weights α at each of 2^n vertices of the n-dimensional cube C_n.

(ii) Observations with weights β at each of $n\,2^{2n-1}$ mid points of the edges of C_n, and

(iii) Observations with weights γ at each of $n(n-1)2^{n-3}$ centers of the two-dimensional faces of C_n,

where $\sum \alpha + \sum \beta + \sum \gamma = 1$. The total number of points in such an experimental design will be

$$2^n + n\,2^{2n-1} + n(n-1)\,2^{n-3} = 2^{n-3}\left[8 + 4n + n(n-1)\right]$$

It is easy to verify that the information matrix given by Eqs. (19), (20) for such a D-Optimal design will have the form

$$M(\xi) = \begin{bmatrix} 1 & u\underline{1}'_n & \underline{0} & \underline{0} \\ u\underline{1}_n & \underline{G} & \underline{0} & \underline{0} \\ \underline{0} & \underline{0} & u\underline{I}_n & \underline{0} \\ \underline{0} & \underline{0} & \underline{0} & \underline{I}\,\binom{n}{2} \end{bmatrix} \tag{47}$$

where

$$\underline{G} = \begin{bmatrix} u & v & v \ldots v \\ v & u & v \ldots v \\ \cdot & & \\ \cdot & & \\ v & v & v \ldots u \end{bmatrix} \tag{48}$$

is a n x n matrix with diagonal elements u and non-diagonal elements ,

$u = \sum_{i=1}^{N} x_{i1}^2 b_i$, b_i is equal to one of the three values

$$\begin{aligned} &= \alpha \binom{n}{0} 2^{n-0} (\pm 1)^2 + \beta\left[0^2 \cdot 2^{n-1} + (\pm 1)^2 \left\{\binom{n}{1} 2^{n-1} - 2^{n-1}\right\}\right] \\ &\quad + \gamma\left[0^2 \cdot (n-1)\,2^{n-2} + \left\{\binom{n}{2} 2^{n-2} - (n-1)\,2^{n-2}\right\}(\pm 1)^2\right] \end{aligned} \tag{49}$$

$$= 2^n \alpha + (n-1)\,2^{n-1}\beta + (n-1)(n-2)\,2^{n-3}\gamma$$

$$= 2^{n-3}\left[8\alpha + 4(n-1)\beta + (n-1)(n-2)\gamma\right]$$

$$= \sum_{i=1}^{N} x_{i1}^2 x_{i2}^2 b_i$$

$$= \alpha \binom{n}{0} 2^{n-0} (\pm 1)^2 (\pm 1)^2 + \beta\left[2^{n-3}(n-2)4\right] + \gamma\left[2^{n-4}(n-2)(n-3)\frac{4}{2!}\right]$$

$$= \alpha 2^n + \beta 2^{n-3}(n-2)4 + \gamma\left[2^{n-3}(n-2)(n-3)\right]$$

$$= 2^{n-3}\left[8\alpha + 4(n-2)\beta + (n-2)(n-3)\gamma\right] \tag{50}$$

The determinant of the matrix $M(\epsilon)$ in (47) is equal to

$$|M(\epsilon)| = u^n v^{n(n-1)/2} (u-v)^{n-1} \left[u + (n-1)v - nu^2\right] \tag{51}$$

as shown below. Writing

$$M(\epsilon) = \begin{bmatrix} \underline{A} & \underline{0} \\ \underline{0} & \underline{B} \end{bmatrix}, \tag{52}$$

where

$$\underline{A} = \begin{bmatrix} 1 & u\underline{1}'_n \\ u\underline{1}_n & \underline{G} \end{bmatrix}, \text{ and} \tag{53}$$

$$\underline{B} = \begin{bmatrix} u\underline{I}_n & \underline{0} \\ \underline{0} & v\underline{I}_{\binom{n}{2}} \end{bmatrix}, \tag{54}$$

$$|M(\epsilon)| = |\underline{A}|\,|\underline{B}| \tag{55}$$

But

$$|\underline{B}| = |u\underline{I}_n|\,|v\underline{I}_{\binom{n}{2}}| \tag{56}$$

$$= u^n v^{n(n-1)/2} \tag{57}$$

and the determinant of the $(n+1) \times (n+1)$ matrix $\underline{A}$ is

$$|\underline{A}| = \begin{vmatrix} 1 & u & u & \cdots & u & u \\ u & u & v & \cdots & v & v \\ u & v & u & \cdots & v & v \\ \vdots & & & & & \\ u & v & v & \cdots & u & v \\ u & v & v & \cdots & v & u \end{vmatrix} = \begin{vmatrix} 1 & u & u & \cdots & u & u \\ 0 & u-v & 0 & \cdots & 0 & -(u-v) \\ 0 & 0 & u-v & \cdots & 0 & -(u-v) \\ \vdots & & & & & \\ 0 & 0 & 0 & \cdots & u-v & -(u-v) \\ u & v & v & \cdots & v & u \end{vmatrix}$$

$$= (u-v)^{n-1} \begin{vmatrix} 1 & u & u & \cdots & u & u \\ 0 & 1 & 0 & \cdots & 0 & -1 \\ 0 & 0 & 1 & \cdots & 0 & -1 \\ \vdots & & & & & \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ u & v & v & \cdots & v & u \end{vmatrix}$$

$$= (u-v)^{n-1}\left\{\begin{vmatrix} 1 & 0 & \cdots & 0 & -1 \\ 0 & 1 & \cdots & 0 & -1 \\ \vdots & & & & \\ 0 & 0 & \cdots & 1 & -1 \\ v & v & \cdots & v & u \end{vmatrix} + (-1)^n u^2 \begin{vmatrix} 1 & 1 & \cdots & 1 & 1 \\ 1 & 0 & \cdots & 0 & -1 \\ 0 & 1 & \cdots & 0 & -1 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & & 1 & -1 \end{vmatrix}\right\}$$

$$= (u-v)^{n-1}\left[u + (n-1)v + (-1)^n u^2 (-1)^{n-3} n\right]$$

(58)

$$= (u-v)^{n-1}\left[u + (n-1)v - 2u^2\right]$$

Substituting from (57) and (58) into (55) we get (51).

The determinant $|M(\epsilon)|$ will attain its maximum value for those values of u and v in (51) which satisfy the system of equations

(59) $$\frac{\partial}{\partial u}|M(\epsilon)| = 0 \qquad \text{and} \qquad \frac{\partial}{\partial v}|M(\epsilon)| = 0$$

or $$2u^2 + 2(n-2)uv - (2n+1)u^3 + (n+2)u^2 v - (n-1)v^2 = 0$$

and $$u^2 + (n-2)uv - nu^3 - (n+1)v^2 + (n+2)u^2 v = 0$$

Solving these equations under the condition $\alpha > 0, \beta > 0, \gamma > 0$, we obtain

(60) $$u = \frac{n+3}{4(n+1)(n+2)^2}\left[2n^2 + 3n + 7 + (n-1)(4n^2+12n+17)^{1/2}\right],$$

(61) $$v = \frac{n+3}{8(n+1)(n+2)^3}\left[4n^3 + 8n^2 + 11n - 5 + (2n^2+n+3)(4n^2+12n+17)^{1/2}\right]$$

The variance-covariance matrix (27) for a quadratic response surface for a D-Optimal design with information matrix given in (47) becomes

(62) $$V(\underline{b}) = \sigma^2 M^{-1}(\epsilon) = \begin{bmatrix} \hat{p}\sigma^2 & \sigma^2 \hat{q}\,\underline{1}_n' & \underline{0} & \underline{0} \\ \sigma^2 \hat{q}\,\underline{1}_n & \sigma^2 \underline{F} & \underline{0} & \underline{0} \\ \underline{0} & \underline{0} & \sigma^2 \hat{u}^{-1} \underline{I}_n & \underline{0} \\ \underline{0} & \underline{0} & & \sigma^2 \hat{v}^{-1} \underline{I}_{\binom{n}{2}} \end{bmatrix}$$

where

$$\hat{p} = \left[u^2 + (n-2)uv - (n-1)v^2\right]T$$

$$\hat{q} = (-1)^{n-1} uT$$

$$\hat{u} = \left[u + (n-2)v - (n-1)u^2\right]T$$

$$\hat{v} = (u^2 - v)T$$

$$T = \left[(u-v)\left\{u + (n-1)v - nu^2\right\}\right]^{-1}$$

and

$$\underline{F} = \begin{bmatrix} \hat{u} & \hat{v} & \hat{v} & \cdots & \hat{v} \\ \hat{v} & \hat{u} & \hat{v} & \cdots & \hat{v} \\ \vdots & & & & \\ \hat{v} & \hat{v} & \hat{v} & \cdots & \hat{u} \end{bmatrix} \quad \text{is} \quad n \times n$$

The orthogonality property for quadratic response surface designs, as given by Eq. (28), requires

$$\sigma^2 (u^2 - v) T = 0$$

which leads to the orthogonality condition

$$u^2 = v \tag{63}$$

because $\sigma^2 \neq 0, T \neq 0$. But the orthogonality condition (63) does not hold for u and v given by Eqs. (60) and (61) respectively, as can easily be verified. Thus we have proved the following important theorem.

Theorem 8. D-Optimal designs for quadratic response are not orthogonal.

7. RECOMMENDATIONS FOR FURTHER STUDY AND INVESTIGATIONS

As already noted before, the validity of the results of the optimization and sensitivity analysis depends heavily on the accuracy of the surface fit approximation procedure. Even for a given experimental design, various estimation procedures for the unknown model coefficients can play an important role in improving the over all accuracy of the response surface approximation and the entire methodology.

The regression analysis currently in use for estimating the regression coefficients in the polynomial approximation of a response surface using any experimental design is what is called least squares estimation. But if the design is not orthogonal, as is the case with D-Optimal designs for quadratic response, the least squares estimates are sensitive to a number of "errors." Sometimes the results of these errors are critical and the least squares estimates even do not make sense when put into the

context of the physics and engineering of the process which is generating the data.

Estimation based on the matrix $(\underline{X}'\underline{X} + k\underline{I})$, $k \geq 0$, rather than on $\underline{X}'\underline{X}$, has been found to be a procedure that can be used to help circumvent many of the difficulties associated with the usual least squares estimates. In particular, the procedure can be used to portray the sensitivity of the estimates to the particular set of data being used, and it can be used to obtain a point estimate with a smaller mean square error. A. E. Hoerl first suggested in 1962 (see reference [6]) that to control the inflation and general instability associated with the least squares estimates, one can use

$$\underline{b}^{*} = \left(\underline{X}'\underline{X} + k\underline{I}\right)^{-1} \underline{X}'\underline{Y} \tag{64}$$

in place of Eq. (13). Estimation and analysis built around (64) has been labeled "ridge regression."

In the light of Theorem 8, which establishes the non-orthogonality of D-Optimal designs for quadratic response, it is strongly suggested that a few case-studies be undertaken to verify the possible superiority of ridge regression analysis for D-Optimal designs for quadratic response.

Also, other optimality criteria should be examined for experimental designs which may lead to orthogonal designs, if possible, for quadratic response.

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